

Butyl ether
142-96-1 | DTXSID1022007

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 69.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 36.3</div> <div>Predicted: 42.5</div>	<div>Image not found</div> <div>1-Nonanol</div> <div>Measured: 77.6</div> <div>Predicted: 101</div>	<div>Image not found</div> <div>Ethyl hexanoate</div> <div>Measured: 115</div> <div>Predicted: 110</div>
<div>Image not found</div> <div>1-Heptanol</div> <div>Measured: 13.8</div> <div>Predicted: 18.6</div>	<div>Image not found</div> <div>Butylbenzene</div> <div>Measured: 2450</div> <div>Predicted: 1580</div>	